Kenneth Ruud

List of Publications by Year
in descending order

335 papers	16,495 citations	16791 66 h-index	26792 111 g-index
364 all docs	364 docs citations	364 times ranked	9253 citing authors

#	Article	IF	Citations
1	Choosing Bad versus Worse: Predictions of Two-Photon-Absorption Strengths Based on Popular Density Functional Approximations. Journal of Chemical Theory and Computation, 2022, 18, 1046-1060.	2.3	26
2	Accurate X-ray Absorption Spectra near L- and M-Edges from Relativistic Four-Component Damped Response Time-Dependent Density Functional Theory. Inorganic Chemistry, 2022, 61, 830-846.	1.9	12
3	Behind the scenes of spin-forbidden decay pathways in transition metal complexes. Physical Chemistry Chemical Physics, 2021, 23, 59-81.	1.3	14
4	Harmonic Infrared and Raman Spectra in Molecular Environments Using the Polarizable Embedding Model. Journal of Chemical Theory and Computation, 2021, 17, 3599-3617.	2.3	6
5	FAIR and transparent research data. Open Science Talk, 2021, , .	0.1	0
6	Demystifying the Origin of Vibrational Coherence Transfer Between the S₁ and T₁ States of the Pt-pop Complex. Journal of Physical Chemistry Letters, 2021, 12, 9768-9773.	2.1	6
7	DORA in practice. Septentrio Conference Series, 2021, , .	0.0	0
8	Relativistic Four-Component DFT Calculations of Vibrational Frequencies. Journal of Physical Chemistry A, 2021, 125, 10315-10320.	1.1	2
9	A generalized few-state model for the first hyperpolarizability. Journal of Chemical Physics, 2020, 152, 244106.	1.2	7
10	Two-photon absorption in host-guest complexes. Molecular Physics, 2020, 118, e1777335.	0.8	3
11	Computational Investigation on the Photophysical Properties of Halogenated Tetraphenyl BODIPY. Journal of Physical Chemistry C, 2020, 124, 11100-11109.	1.5	5
12	ReSpect: Relativistic spectroscopy DFT program package. Journal of Chemical Physics, 2020, 152, 184101.	1.2	90
13	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
14	Arctic Advanced Education and Research. , 2020, , 133-141.		0
15	Opening speech for the 15th Munin Conference on Scholarly Publishing 2020. Septentrio Conference Series, 2020, , .	0.0	0
16	Implementing DORA. Open Science Talk, 2020, , .	0.1	0
17	Photo-Transformation Trajectories of Nitro-Spiropyran in Hybrid Compounds with [60]Fullerene. Journal of Physical Chemistry C, 2019, 123, 18215-18221.	1.5	3
18	All-electron fully relativistic Kohn-Sham theory for solids based on the Dirac-Coulomb Hamiltonian and Gaussian-type functions. Physical Review B, 2019, 99, .	1.1	24

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19	Relativistic four-component linear damped response TDDFT for electronic absorption and circular dichroism calculations. Journal of Chemical Physics, 2019, 151, 194112.	1.2	17
20	Strong Duschinsky Mixing Induced Breakdown of Kashaâ€™s Rule in an Organic Phosphor. Journal of Physical Chemistry Letters, 2019, 10, 369-374.	2.1	28
21	Electron-Spin Structure and Metalâ€“Ligand Bonding in Open-Shell Systems from Relativistic EPR and NMR: A Case Study of Square-Planar Iridium Catalysts. Journal of Chemical Theory and Computation, 2019, 15, 201-214.	2.3	17
22	Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde. Journal of Chemical Theory and Computation, 2018, 14, 1333-1350.	2.3	41
23	Darmstadtium, roentgenium, and copernicium form strong bonds with cyanide. International Journal of Quantum Chemistry, 2018, 118, e25393.	1.0	9
24	Insight into the fluorescence quenching of Trp214 at HSA by the Dimetridazole ligand from simulation. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 354, 86-100.	2.0	7
25	Resolution-of-identity accelerated relativistic two- and four-component electron dynamics approach to chiroptical spectroscopies. Journal of Chemical Physics, 2018, 149, 204104.	1.2	23
26	An efficient pseudo-spectral method for the description of atomic electronic wave functions â€“ Application to the hydrogen atom in a uniform magnetic field. Chemical Physics, 2018, 515, 299-314.	0.9	1
27	Rare and Nonexistent Nitrosyls: Periodic Trends and Relativistic Effects in Ruthenium and Osmium Porphyrin-Based {MNO}⁷ Complexes. ACS Omega, 2018, 3, 10513-10516.	1.6	10
28	Benchmarking the Performance of Exchange-Correlation Functionals for Predicting Two-Photon Absorption Strengths. Journal of Chemical Theory and Computation, 2018, 14, 3677-3685.	2.3	56
29	Unraveling the Microscopic Origin of Triplet Lasing from Organic Solids. Journal of Physical Chemistry Letters, 2018, 9, 4314-4318.	2.1	9
30	Implementing DORA at UiT The Arctic University of Norway. Septentrio Conference Series, 2018, , .	0.0	0
31	Molecular Electric, Magnetic, and Optical Properties. , 2017, , 497-592.		5
32	Origin of Dual-Peak Phosphorescence and Ultralong Lifetime of 4,6-Diethoxy-2-carbazolyl-1,3,5-triazine. Journal of Physical Chemistry Letters, 2017, 8, 1253-1258.	2.1	22
33	Interplay of twist angle and solvents with two-photon optical channel interference in aryl-substituted BODIPY dyes. Physical Chemistry Chemical Physics, 2017, 19, 29461-29471.	1.3	11
34	Anomalous Phosphorescence from an Organometallic White-Light Phosphor. Journal of Physical Chemistry Letters, 2017, 8, 4893-4897.	2.1	17
35	Cryptophanes for Methane and Xenon Encapsulation: A Comparative Density Functional Theory Study of Binding Properties and NMR Chemical Shifts. Journal of Physical Chemistry A, 2017, 121, 9669-9677.	1.1	8
36	Channel interference in multiphoton absorption. Journal of Chemical Physics, 2017, 146, 244116.	1.2	16

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37	Gauge-origin independent calculations of electric-field-induced second-harmonic generation circular intensity difference using London atomic orbitals. Molecular Physics, 2017, 115, 241-251.	0.8	5
38	Open-ended formulation of self-consistent field response theory with the polarizable continuum model for solvation. Physical Chemistry Chemical Physics, 2017, 19, 366-379.	1.3	5
39	Four-component relativistic density functional theory with the polarisable continuum model: application to EPR parameters and paramagnetic NMR shifts. Molecular Physics, 2017, 115, 214-227.	0.8	21
40	Relativistic Theory of Nuclear Spin-Rotation Tensor. , 2017, , 693-723.		2
41	Institutional transformation towards Open Science: Experiences from UiT The Arctic University of Norway. Septentrio Conference Series, 2017, , .	0.0	0
42	NMR absolute shielding scale and nuclear magnetic dipole moment of ²⁰⁷Pb. Physical Chemistry Chemical Physics, 2016, 18, 16483-16490.	1.3	23
43	Indirect NMR spinâ€“spin coupling constants in diatomic alkali halides. Journal of Chemical Physics, 2016, 145, 244308.	1.2	7
44	Magnetic properties with multiwavelets and DFT: the complete basis set limit achieved. Physical Chemistry Chemical Physics, 2016, 18, 21145-21161.	1.3	40
45	Mercury Methylation by Cobalt Corrinoids: Relativistic Effects Dictate the Reaction Mechanism. Angewandte Chemie, 2016, 128, 11675-11678.	1.6	4
46	Open-ended response theory with polarizable embedding: multiphoton absorption in biomolecular systems. Physical Chemistry Chemical Physics, 2016, 18, 28339-28352.	1.3	23
47	Mercury Methylation by Cobalt Corrinoids: Relativistic Effects Dictate the Reaction Mechanism. Angewandte Chemie - International Edition, 2016, 55, 11503-11506.	7.2	33
48	Chiral recognition by fullerenes: CHFClBr enantiomers in the C82cage. Physical Chemistry Chemical Physics, 2016, 18, 26057-26068.	1.3	12
49	Complete analytic anharmonic hyper-Raman scattering spectra. Physical Chemistry Chemical Physics, 2016, 18, 22331-22342.	1.3	5
50	Acceleration of Relativistic Electron Dynamics by Means of X2C Transformation: Application to the Calculation of Nonlinear Optical Properties. Journal of Chemical Theory and Computation, 2016, 12, 5823-5833.	2.3	48
51	Structure, NMR and Electronic Spectra of [m.n]Paracyclophanes with Varying Bridges Lengths (m, n = 2â€“4). Journal of Physical Chemistry A, 2016, 120, 724-736.	1.1	10
52	Three-photon circular dichroism: towards a generalization of chiroptical non-linear light absorption. Physical Chemistry Chemical Physics, 2016, 18, 4174-4184.	1.3	10
53	Analytic calculations of anharmonic infrared and Raman vibrational spectra. Physical Chemistry Chemical Physics, 2016, 18, 4201-4215.	1.3	27
54	Absolute NMR shielding scales and nuclear spinâ€“rotation constants in 175LuX and 197AuX (X = 19F,) Tj ETQq0 0 0 rgBT /Overlock 10	1.2	18

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55	Experimental and fourâ€component relativistic DFT studies of tungsten carbonyl complexes. Journal of Physical Organic Chemistry, 2015, 28, 723-731.	0.9	17
56	Pyrrolo[3,2â€b]pyrrolesâ€"From Unprecedented Solvatofluorochromism to Twoâ€Photon Absorption. Chemistry - A European Journal, 2015, 21, 18364-18374.	1.7	93
57	FemExâ€"female excellence in theoretical and computational chemistry. International Journal of Quantum Chemistry, 2015, 115, 1195-1196.	1.0	3
58	The origin dependence of the material constants: the permittivity and the inverse permeability. Molecular Physics, 2015, 113, 1899-1913.	0.8	7
59	NMR shielding and spinâ€"rotation constants in XCO (X = Ni, Pd, Pt) molecules. Molecular Physics, 2015, 113, 1576-1584.	0.8	19
60	Open-Ended Recursive Calculation of Single Residues of Response Functions for Perturbation-Dependent Basis Sets. Journal of Chemical Theory and Computation, 2015, 11, 4814-4824.	2.3	5
61	Four-Component Relativistic Density Functional Theory Calculations of EPRg- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spinâ€"Orbit Effects. Journal of Physical Chemistry A, 2015, 119, 12892-12905.	1.1	49
62	Polarizable Density Embedding: A New QM/QM/MM-Based Computational Strategy. Journal of Physical Chemistry A, 2015, 119, 5344-5355.	1.1	78
63	Excitation Energies from Real-Time Propagation of the Four-Component Diracâ€"Kohnâ€"Sham Equation. Journal of Chemical Theory and Computation, 2015, 11, 980-991.	2.3	72
64	Open-Ended Recursive Approach for the Calculation of Multiphoton Absorption Matrix Elements. Journal of Chemical Theory and Computation, 2015, 11, 1129-1144.	2.3	35
65	Molecular quantum mechanical gradients within the polarizable embedding approachâ€"Application to the internal vibrational Stark shift of acetophenone. Journal of Chemical Physics, 2015, 142, 034119.	1.2	17
66	Benchmarking two-photon absorption cross sections: performance of CC2 and CAM-B3LYP. Physical Chemistry Chemical Physics, 2015, 17, 19306-19314.	1.3	160
67	Four-Component Relativistic Density-Functional Theory Calculations of Nuclear Spinâ€"Rotation Constants: Relativistic Effects in p-Block Hydrides. Journal of Chemical Theory and Computation, 2015, 11, 3729-3739.	2.3	32
68	Five-Photon Absorption and Selective Enhancement of Multiphoton Absorption Processes. ACS Photonics, 2015, 2, 572-577.	3.2	16
69	X-ray absorption resonances near L_{2,3}-edges from real-time propagation of the Diracâ€"Kohnâ€"Sham density matrix. Physical Chemistry Chemical Physics, 2015, 17, 22566-22570.	1.3	58
70	Structure, solvent, and relativistic effects on the NMR chemical shifts in square-planar transition-metal complexes: assessment of DFT approaches. Physical Chemistry Chemical Physics, 2015, 17, 24944-24955.	1.3	82
71	DFT as a Powerful Predictive Tool in Photoredox Catalysis: Redox Potentials and Mechanistic Analysis. Organometallics, 2015, 34, 4218-4228.	1.1	57
72	Communication: The absolute shielding scales of oxygen and sulfur revisited. Journal of Chemical Physics, 2015, 142, 091102.	1.2	27

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73	Molecular Electric, Magnetic, and Optical Properties. , 2015, , 1-97.		2
74	Relativistic Theory of Nuclear Spin-Rotation Tensor. , 2015, , 1-31.		0
75	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	1.5	22
76	Analytic calculations of hyper-Raman spectra from density functional theory hyperpolarizability gradients. Journal of Chemical Physics, 2014, 141, 134107.	1.2	12
77	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
78	Intermolecular charge transfer enhances two-photon absorption in yellow fluorescent protein. Physical Chemistry Chemical Physics, 2014, 16, 5958.	1.3	46
79	Spin-Rotation and NMR Shielding Constants in XF Molecules (X = B, Al, Ga, In, and Tl). Journal of Physical Chemistry A, 2014, 118, 9588-9595.	1.1	15
80	A general, recursive, and openâ€ended response code. Journal of Computational Chemistry, 2014, 35, 622-633.	1.5	34
81	Analytic cubic and quartic force fields using density-functional theory. Journal of Chemical Physics, 2014, 140, 034103.	1.2	38
82	Analytic Density Functional Theory Calculations of Pure Vibrational Hyperpolarizabilities: The First Dipole Hyperpolarizability of Retinal and Related Molecules. Journal of Physical Chemistry A, 2014, 118, 748-756.	1.1	6
83	Cob(II)alamin: Relativistic DFT Analysis of the EPR Parameters. Journal of Chemical Theory and Computation, 2014, 10, 2125-2136.	2.3	12
84	Chemical Control of Channel Interference in Two-Photon Absorption Processes. Accounts of Chemical Research, 2014, 47, 1604-1612.	7.6	59
85	Ab initio and relativistic DFT study of spinâ€“rotation and NMR shielding constants in XF6 molecules, X = S, Se, Te, Mo, and W. Journal of Chemical Physics, 2014, 140, 194308.	1.2	35
86	Theoretical investigation of two model systems for molecular photoswitch functionality. I. 2-(4-nitropyrimidin-2-yl)ethenol. Molecular Physics, 2014, 112, 818-835.	0.8	1
87	Convergence of environment polarization effects in multiscale modeling of excitation energies. Computational and Theoretical Chemistry, 2014, 1040-1041, 304-311.	1.1	36
88	Shape-Dependent Electronic Excitations in Metallic Chains. Journal of Physical Chemistry C, 2014, 118, 13059-13069.	1.5	10
89	Rotational averaging of multiphoton absorption cross sections. Journal of Chemical Physics, 2014, 141, 204103.	1.2	30
90	Effect of donorâ€“acceptor orientation on solvent-dependent three-photon activity in through-space charge-transfer systems â€“ case study of [2,2]-paracyclophane derivatives. Physical Chemistry Chemical Physics, 2013, 15, 17570.	1.3	7

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91	Four-Component Relativistic Density Functional Theory Calculations of NMR Shielding Tensors for Paramagnetic Systems. Journal of Physical Chemistry A, 2013, 117, 14209-14219.	1.1	60
92	All-Metal Aromaticity: Revisiting the Ring Current Model among Transition Metal Clusters. Journal of Chemical Theory and Computation, 2013, 9, 4789-4796.	2.3	90
93	The Absolute Shielding Constants of Heavy Nuclei: Resolving the Enigma of the ¹¹⁹Sn Absolute Shielding. Journal of Physical Chemistry Letters, 2013, 4, 459-463.	2.1	64
94	Cob(I)alamin: Insight Into the Nature of Electronically Excited States Elucidated via Quantum Chemical Computations and Analysis of Absorption, CD and MCD Data. Journal of Physical Chemistry A, 2013, 117, 863-876.	1.1	24
95	A polarizable embedding DFT study of one-photon absorption in fluorescent proteins. Physical Chemistry Chemical Physics, 2013, 15, 4735.	1.3	44
96	Determination of Absolute Configuration and Conformation of a Cyclic Dipeptide by NMR and Chiral Spectroscopic Methods. Journal of Physical Chemistry A, 2013, 117, 1721-1736.	1.1	59
97	Multiconfigurational Self-Consistent Field Calculations of the Magnetically Induced Current Density Using Gauge-Including Atomic Orbitals. Journal of Chemical Theory and Computation, 2013, 9, 2189-2198.	2.3	34
98	Fully adaptive algorithms for multivariate integral equations using the non-standard form and multiwavelets with applications to the Poisson and bound-state Helmholtz kernels in three dimensions. Molecular Physics, 2013, 111, 1143-1160.	0.8	37
99	Fourâ€component relativistic chemical shift calculations of halogenated organic compounds. Journal of Physical Organic Chemistry, 2013, 26, 679-687.	0.9	19
100	First Principles Studies of the Vibrationally Resolved Magnetic Circular Dichroism Spectra of Biphenylene. Journal of Chemical Theory and Computation, 2013, 9, 1557-1567.	2.3	19
101	Effective time-independent studies on resonance Raman spectroscopy of trans-stilbene including the Duschinsky effect. Molecular Physics, 2013, 111, 1511-1525.	0.8	4
102	Role of zero-point vibrational corrections to carbon hyperfine coupling constants in organic Ï€ radicals. Journal of Chemical Physics, 2013, 138, 054310.	1.2	6
103	Analytic evaluation of the dipole Hessian matrix in coupled-cluster theory. Journal of Chemical Physics, 2013, 139, 154106.	1.2	6
104	Spin-rotation and NMR shielding constants in HCl. Journal of Chemical Physics, 2013, 139, 234302.	1.2	25
105	Plasmon resonances in linear noble-metal chains. Journal of Chemical Physics, 2012, 137, 194307.	1.2	35
106	Hyper Raman spectra calculated in a time-dependent Hartreeâ€“Fock method. Molecular Physics, 2012, 110, 2315-2320.	0.8	5
107	A general toolbox for the calculation of higher-order molecular properties using SCF wave functions at the one-, two- and four-component levels of theory. , 2012, , .		0
108	Porphyrin Protonation Studied by Magnetic Circular Dichroism. Journal of Physical Chemistry A, 2012, 116, 778-783.	1.1	32

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109	Transferability of Various Molecular Property Tensors in Vibrational Spectroscopy. Journal of Chemical Theory and Computation, 2012, 8, 977-985.	2.3	60
110	A Combined Atomic Force Microscopy and Computational Approach for the Structural Elucidation of Breitfussin A and B: Highly Modified Halogenated Dipeptides from Thuiaria breitfussi. Angewandte Chemie - International Edition, 2012, 51, 12238-12241.	7.2	92
111	Calculation of two-photon absorption strengths with the approximate coupled cluster singles and doubles model CC2 using the resolution-of-identity approximation. Physical Chemistry Chemical Physics, 2012, 14, 1175-1184.	1.3	76
112	Charge-Transfer Excitations in Uranyl Tetrachloride ([UO₂Cl₄]^{2â€“}): How Reliable are Electronic Spectra from Relativistic Time-Dependent Density Functional Theory?. Journal of Physical Chemistry A, 2012, 116, 7397-7404.	1.1	47
113	A combined quantum mechanics/molecular mechanics study of the one- and two-photon absorption in the green fluorescent protein. Physical Chemistry Chemical Physics, 2012, 14, 5440.	1.3	76
114	Vibrationally resolved circular dichroism spectra of a molecule with isotopically engendered chirality. Physical Chemistry Chemical Physics, 2012, 14, 3669.	1.3	10
115	Absolute Configuration of a Cyclic Dipeptide Reflected in Vibrational Optical Activity: Ab Initio and Experimental Investigation. Journal of Physical Chemistry A, 2012, 116, 2554-2563.	1.1	30
116	High-Polarity Solvents Decreasing the Two-Photon Transition Probability of Through-Space Charge-Transfer Systems â€” A Surprising In Silico Observation. Journal of Physical Chemistry Letters, 2012, 3, 961-966.	2.1	38
117	Efficient Calculation of ROA Tensors with Analytical Gradients and Fragmentation. Chirality, 2012, 24, 1018-1030.	1.3	15
118	Parallelization of the polarizable embedding scheme for higher-order response functions. Molecular Physics, 2012, 110, 2579-2586.	0.8	2
119	Determining the Absolute Configuration of Two Marine Compounds Using Vibrational Chiroptical Spectroscopy. Journal of Organic Chemistry, 2012, 77, 858-869.	1.7	71
120	Ab initio calculation of magnetic circular dichroism. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 443-455.	6.2	27
121	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. Chemical Reviews, 2012, 112, 543-631.	23.0	549
122	Structure and NMR spectra of cyclophanes with unsaturated bridges (cyclophenes). Magnetic Resonance in Chemistry, 2012, 50, 449-457.	1.1	4
123	Molecular Electric, Magnetic, and Optical Properties. , 2012, , 361-441.		13
124	Zero-point vibrational corrections to isotropic hyperfine coupling constants in polyatomic molecules. Physical Chemistry Chemical Physics, 2011, 13, 696-707.	1.3	14
125	The optical activity of Î²,Î³-enones in ground and excited states using circular dichroism and circularly polarized luminescence. Physical Chemistry Chemical Physics, 2011, 13, 643-650.	1.3	45
126	Electronically Excited States of Vitamin B₁₂ and Methylcobalamin: Theoretical Analysis of Absorption, CD, and MCD Data. Journal of Physical Chemistry B, 2011, 115, 737-748.	1.2	43

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127	Electronically Excited States of Vitamin B₁₂: Benchmark Calculations Including Time-Dependent Density Functional Theory and Correlated ab Initio Methods. Journal of Physical Chemistry A, 2011, 115, 1280-1292.	1.1	94
128	Excitation Energies in Solution: The Fully Polarizable QM/MM/PCM Method. Journal of Physical Chemistry B, 2011, 115, 3027-3037.	1.2	118
129	Explicit versus Implicit Solvent Modeling of Raman Optical Activity Spectra. Journal of Physical Chemistry B, 2011, 115, 4128-4137.	1.2	92
130	The ab initio calculation of molecular electric, magnetic and geometric properties. Physical Chemistry Chemical Physics, 2011, 13, 2627-2651.	1.3	58
131	Structure and NMR Spectra of Some [2.2]Paracyclophanes. The Dilemma of [2.2]Paracyclophane Symmetry. Journal of Physical Chemistry A, 2011, 115, 10638-10649.	1.1	30
132	The First and Second Static Electronic Hyperpolarizabilities of Zigzag Boron Nitride Nanotubes. An ab Initio Approach through the Coupled Perturbed Kohnâ€“Sham Scheme. Journal of Physical Chemistry A, 2011, 115, 12631-12637.	1.1	31
133	Relativistic four-component calculations of Buckingham birefringence using London atomic orbitals. Theoretical Chemistry Accounts, 2011, 129, 685-699.	0.5	4
134	GEN1INT: A unified procedure for the evaluation of one-electron integrals over Gaussian basis functions and their geometric derivatives. International Journal of Quantum Chemistry, 2011, 111, 858-872.	1.0	43
135	Differences in Twoâ€Photon and Oneâ€Photon Absorption Profiles Induced by Vibronic Coupling: The Case of Dioxaborine Heterocyclic Dye. ChemPhysChem, 2011, 12, 3392-3403.	1.0	22
136	Coupledâ€Cluster Calculations of Vibrational Raman Optical Activity Spectra. ChemPhysChem, 2011, 12, 3442-3448.	1.0	34
137	Gauge-origin independent calculations of Jones birefringence. Journal of Chemical Physics, 2011, 135, 134114.	1.2	8
138	Calculation of the first static hyperpolarizability tensor of three-dimensional periodic compounds with a local basis set: A comparison of LDA, PBE, PBE0, B3LYP, and HF results. Journal of Chemical Physics, 2010, 132, 244106.	1.2	68
139	Arbitrary-Order Density Functional Response Theory from Automatic Differentiation. Journal of Chemical Theory and Computation, 2010, 6, 1971-1980.	2.3	174
140	Ab initio study of coherent anti-Stokes Raman scattering (CARS) of the 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) explosive. Chemical Physics Letters, 2010, 485, 320-325.	1.2	6
141	The aqueous Raman optical activity spectra of 4(R)â€hydroxyproline: theory and experiment. Journal of Raman Spectroscopy, 2010, 41, 1200-1210.	1.2	16
142	Excited-state polarizabilities of solvated molecules using cubic response theory and the polarizable continuum model. Journal of Chemical Physics, 2010, 132, 024107.	1.2	8
143	Solvatochromic shift of phenol blue in water from a combined Carâ€“Parrinello molecular dynamics hybrid quantum mechanics-molecular mechanics and <scp>ZINDO</scp> approach. Journal of Chemical Physics, 2010, 132, 234508.	1.2	25
144	Computational Study of the One- and Two-Photon Absorption and Circular Dichroism of (<scp>l</scp>)-Tryptophan. Journal of Physical Chemistry B, 2010, 114, 6500-6512.	1.2	45

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145	An Atomic-Orbital-Based Lagrangian Approach for Calculating Geometric Gradients of Linear Response Properties. Journal of Chemical Theory and Computation, 2010, 6, 1028-1047.	2.3	28
146	Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations. Journal of Chemical Physics, 2009, 131, 144104.	1.2	60
147	Theoretical approaches to the calculation of Raman optical activity spectra. Chirality, 2009, 21, E54-67.	1.3	97
148	Spatial structure and NMR spectra of strained [2.2.2]cyclophanes. Magnetic Resonance in Chemistry, 2009, 47, 407-414.	1.1	5
149	Atomic orbital-based cubic response theory for one-, two-, and four-component relativistic self-consistent field models. Chemical Physics, 2009, 356, 177-186.	0.9	18
150	Synthesis, characterization and assignment of the absolute configuration of 4,4-dimethyl-5-oxo-tetrahydrofuran-3-carboxylic acid and its esters: a combined experimental and theoretical investigation. Tetrahedron: Asymmetry, 2009, 20, 1459-1467.	1.8	7
151	Jones and magnetoelectric birefringence of pure substances â€" A computational study. Canadian Journal of Chemistry, 2009, 87, 1352-1361.	0.6	5
152	Large two-photon absorption cross section: molecular tweezer as a new promising class of compounds for nonlinear optics. Physical Chemistry Chemical Physics, 2009, 11, 2592.	1.3	46
153	Intermolecular Interaction-Controlled Tuning of the Two-Photon Absorption of Fullerene Bound in a Buckycatcher. Journal of Physical Chemistry A, 2009, 113, 5485-5488.	1.1	41
154	On the importance of vibrational contributions to small-angle optical rotation: Fluoro-oxirane in gas phase and solution. Journal of Chemical Physics, 2009, 130, 034310.	1.2	43
155	Analytic calculations of nonlinear mixed electric and magnetic frequency-dependent molecular properties using London atomic orbitals: Buckingham birefringence. Physical Chemistry Chemical Physics, 2009, 11, 816-825.	1.3	14
156	Analytic ab initio calculations of coherent anti-Stokes Raman scattering (CARS). Physical Chemistry Chemical Physics, 2009, 11, 2293.	1.3	19
157	TDDFT diagnostic testing and functional assessment for triazene chromophores. Physical Chemistry Chemical Physics, 2009, 11, 4465.	1.3	145
158	Determination of Molecular Structure of Bisphenylene Homologues of BINOL-Based Phosphoramidites by Chiroptical Methods. Journal of Physical Chemistry A, 2009, 113, 10717-10725.	1.1	17
159	The use of Coulomb-attenuated methods for the calculation of electronic circular dichroism spectra. Chemical Physics, 2008, 349, 234-243.	0.9	39
160	An IEF-PCM study of solvent effects on the Faraday $${mathcal{B}}$$ term of MCD. Theoretical Chemistry Accounts, 2008, 119, 231-244.	0.5	31
161	Solvent effects on zero-point vibrational corrections to optical rotations and nuclear magnetic resonance shielding constants. Chemical Physics Letters, 2008, 451, 226-232.	1.2	50
162	Importance of backbone angles versus amino acid configurations in peptide vibrational Raman optical activity spectra. Chemical Physics, 2008, 343, 200-209.	0.9	32

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163	A density matrix-based quasienergy formulation of the Kohnâ€“Sham density functional response theory using perturbation- and time-dependent basis sets. Journal of Chemical Physics, 2008, 129, 214108.	1.2	99
164	The A and B Terms of Magnetic Circular Dichroism Revisited. Journal of Physical Chemistry A, 2008, 112, 9615-9618.	1.1	55
165	Solvent Effects on the Three-Photon Absorption of a Symmetric Charge-Transfer Molecule. Journal of Physical Chemistry B, 2008, 112, 4703-4710.	1.2	15
166	Degenerate Perturbation Theory for Electronic g Tensors: Leading-Order Relativistic Effects. Journal of Chemical Theory and Computation, 2008, 4, 1810-1828.	2.3	20
167	Analytic Calculations of Vibrational Hyperpolarizabilities in the Atomic Orbital Basis. Journal of Physical Chemistry A, 2008, 112, 11942-11950.	1.1	30
168	Complex polarization propagator calculations of magnetic circular dichroism spectra. Journal of Chemical Physics, 2008, 128, 094103.	1.2	63
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